Porting COSMO to Hybrid Architectures

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Programming weather, climate and earth-system models
on heterogeneous multi-core platforms
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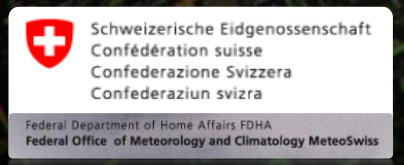
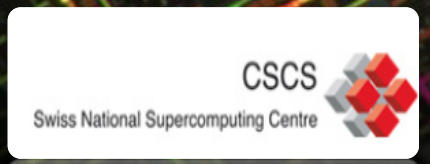


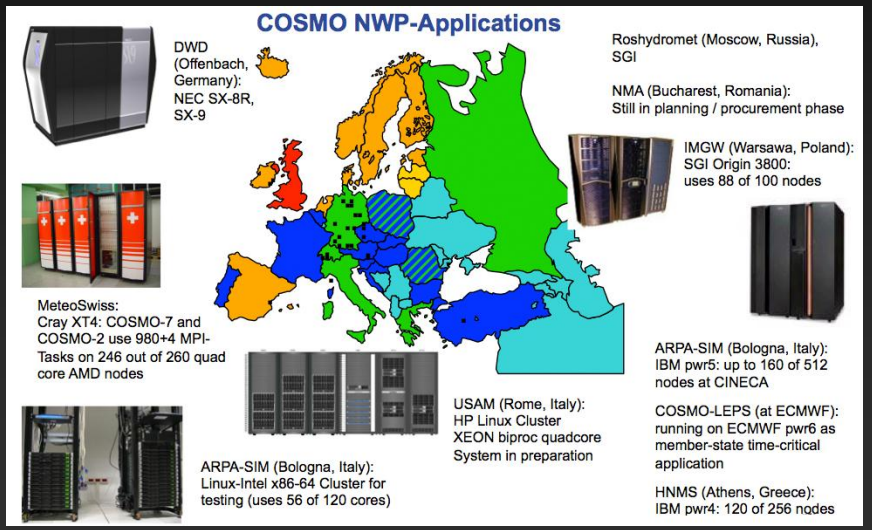


Why Improving COSMO?

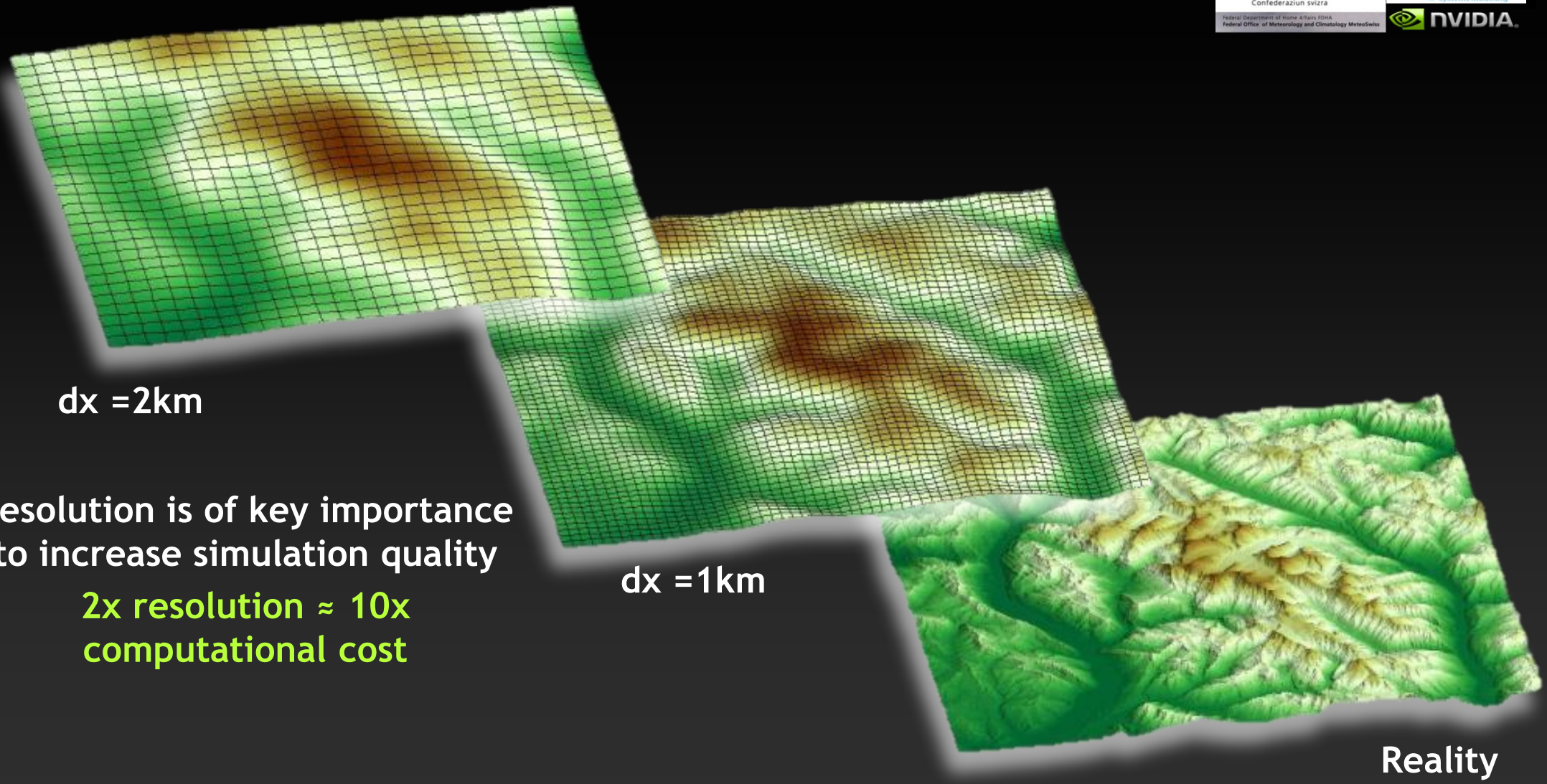
- COSMO: Consortium for Small-Scale Modeling
- Limited-area climate model - http://www.cosmo-model.org/
- Used by 7 weather services and O(50) universities and research institutes

- High CPU usage @ CSCS (Swiss National Supercomputing Center)
  - 30 Mio CPU hours in total
  - ~ 50% on a dedicated machine
- Strong desire for improved simulation quality
  - Higher resolution
  - Larger ensemble simulations
  - Increasing model complexity

→ Performance improvements are critical!



Need for Higher Resolution in Switzerland



Resolution is of key importance to increase simulation quality

2x resolution ≈ 10x computational cost

COSMO port to hybrid architectures is part of HP2C Project

- Part of the Swiss HPCN strategy (hardware / infrastructure / software)
- Strong focus on hybrid architectures for real world applications
- 10 Projects from different domains - http://www.hp2c.ch/
  - **Cardiovascular simulation (EPFL)**
  - **Stellar explosions (University of Basel)**
  - **Quantum dynamics (University of Geneva)**
  - **…**
  - **COSMO-CCLM**
    1. **Cloud resolving climate simulations (IPCC AR5)**
    2. **Adapt existing code (hybrid, I/O)**
    3. **Aggressive developments (different programming languages, GPUs)**

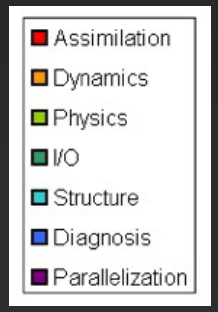
Refactoring Approach

Physics

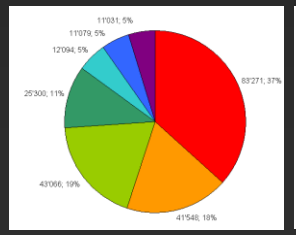
- Large group of developers
- Plug-in code from other models
- Less memory bandwidth bound
- Simpler stencils (K-dependencies)
- 20% of runtime

→ Keep source code (Fortran)

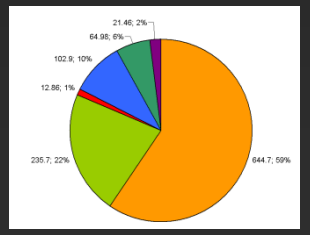
→ GPU port with directives (OpenACC)



Lines of Code



Runtime



Dynamics

- Small group of developers
- Memory bandwidth bound
- Complex stencils (IJK-dependencies)
- 60% of runtime

→ Aggressive rewrite in C++

→ Development of a stencil library

→ Still single source code multiple library back-ends for x86 / GPU

Requirements for a Portable Stencil Library

```
DO k = 1, ke
  DO j = jstart, jend
    DO i = istart, iend
      lap(i,j,k) = data(i+1,j,k)+data(i-1,j,k)+data(i,j+1,k)+data(i,j-1,k) - 4.0*data(i,j,k)
    ENDDO
  ENDDO
ENDDO
```

loop-logic

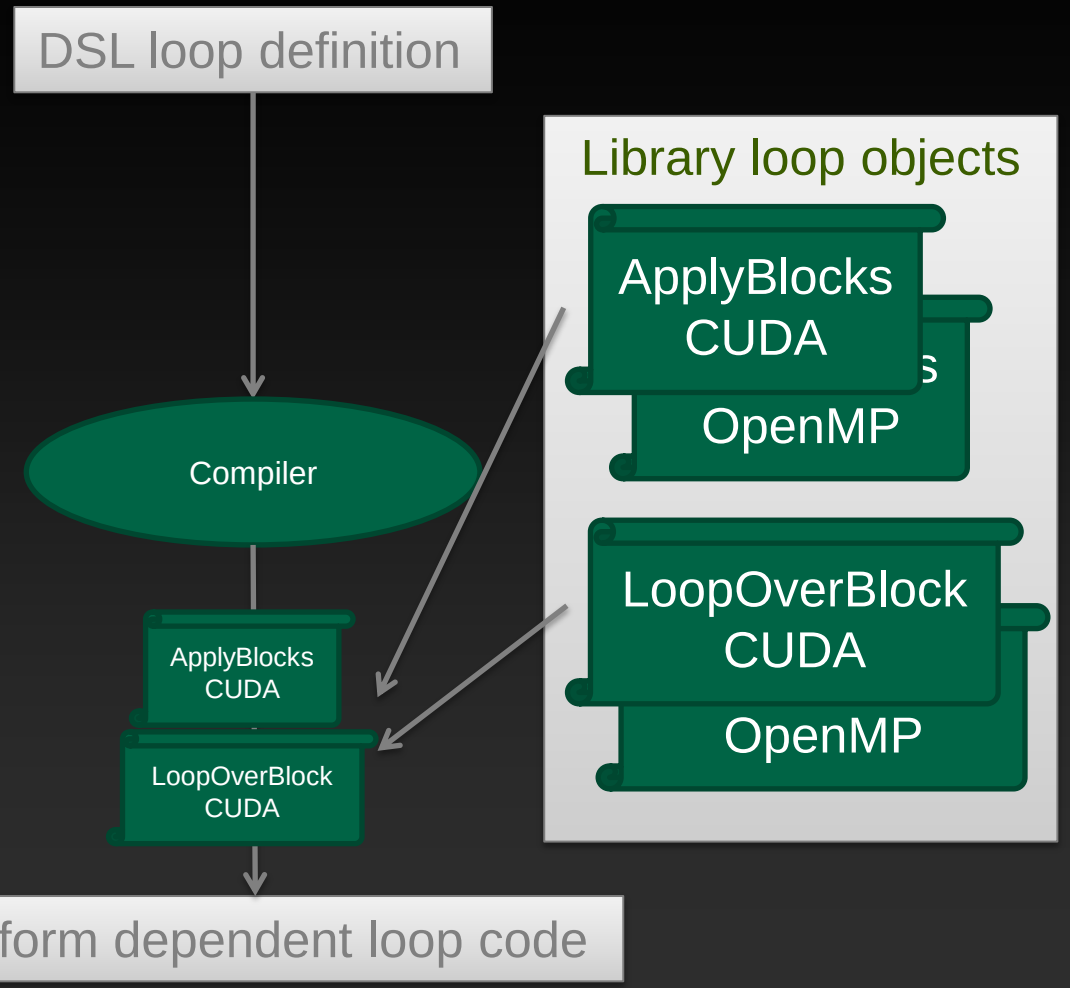
update-function / stencil

- Loop-logic: Defines stencil application domain
  - Platform dependent
- Update-function: Expression evaluated at each location
  - Platform independent

=> Treat two components separately

Loop-Logic expressed in Domain Specific Language (DSL)

- Define embedded domain specific language in C++ using type system/template metaprogramming
  - Code is written as type
  - Type is translated into sequence of operations (DSL compilation) at compile time
  - Operation objects (“code fragments”) are inserted at compile time (code generation)
- Pre-packaged loop objects for CPU and GPU
- We use this approach to generate the platform dependent loop-logic



Putting it all together..

```
IJKRealField laplacian, pressure;
Stencil stencil;
StencilCompiler::Build(
  stencil,
  "Example",
  calculationDomainSize,
  StencilConfiguration<Real, BlockSize<32,4> >(),
  ….

    define_sweep<KLoopFullDomain>(
      define_stages(
        StencilStage<LapStage, IJBoundary<cComplete,0,0,0,0> >()
      )
    )

);

stencil.Apply();
```

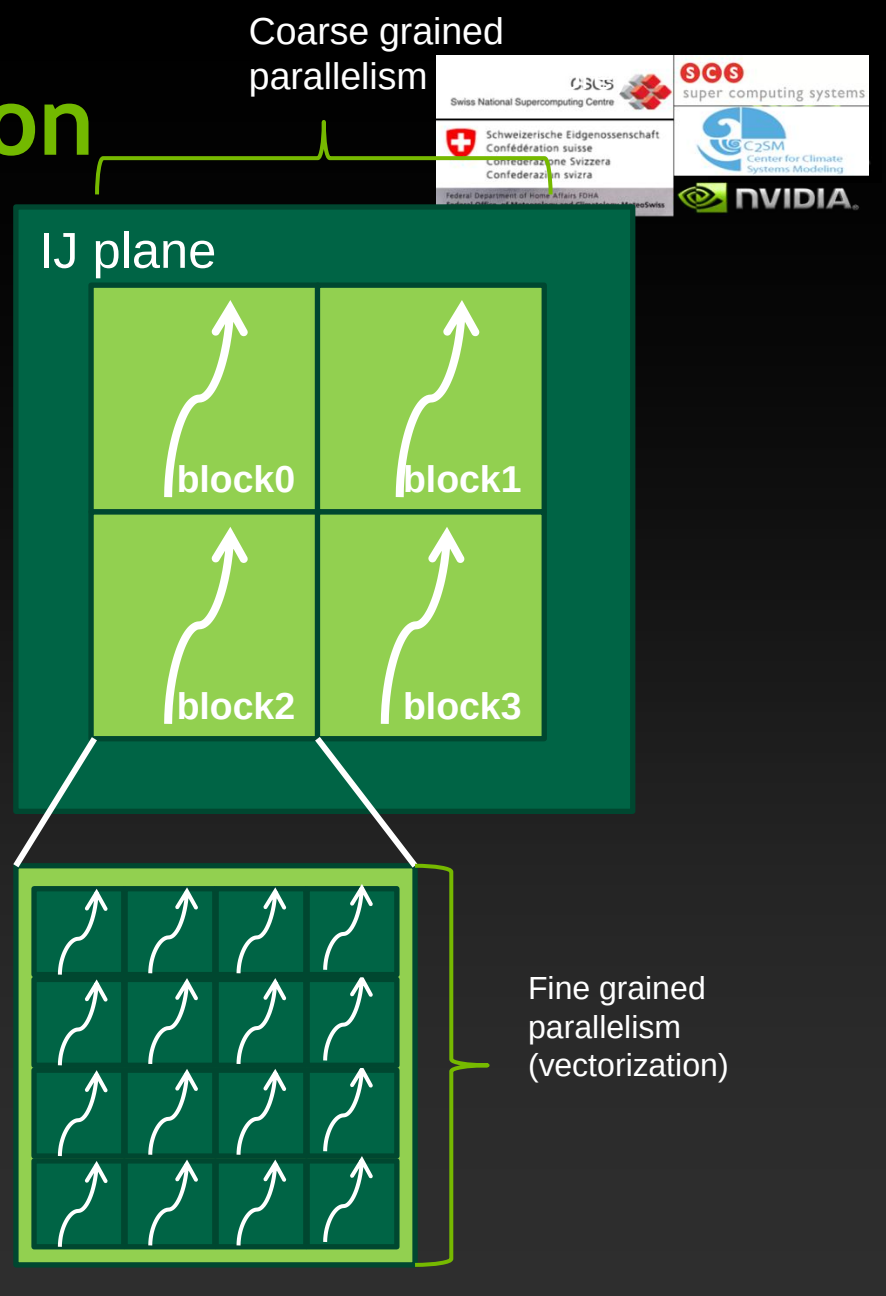
```
DO k = 1, ke
  DO j = jstart, jend
    DO i = istart, iend
      lap(i,j,k) = data(i+1,j,k) + …
    ENDDO
  ENDDO
ENDDO
```

```
enum { data, lap };

template<typename TEnv>
struct LapStage
{
  STENCIL_STAGE(TEnv)

  STAGE_PARAMETER(FullDomain, data)
  STAGE_PARAMETER(FullDomain, lap)

  static void Do(Context ctx, FullDomain)
  {
    ctx[lap::Center()] =
      -4.0 * ctx[data::Center()] +
      ctx[data::At(iplus1)] +
      ctx[data::At(iminus1)] +
      ctx[data::At(jplus1)] +
      ctx[data::At(jminus1)];
  }
};
```

Stencil Library Parallelization

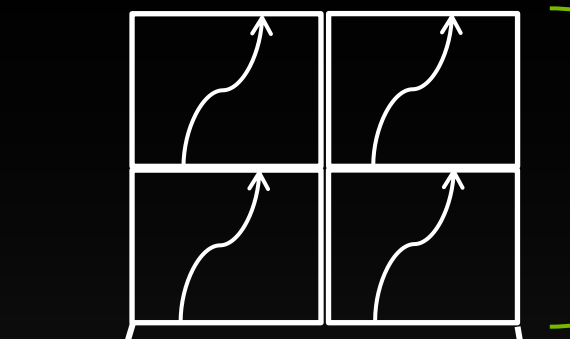
- Shared memory parallelization
  - Support for 2 levels of parallelism
- Coarse grained parallelism
  - Split domain into blocks
  - Distribute blocks to CPU cores
  - No synchronization & consistency required
- Fine grained parallelism
  - Update block on a single core
  - Lightweight threads / vectors
  - Synchronization & consistency required

~ CUDA programming model
(should be a good match for other platforms as well)

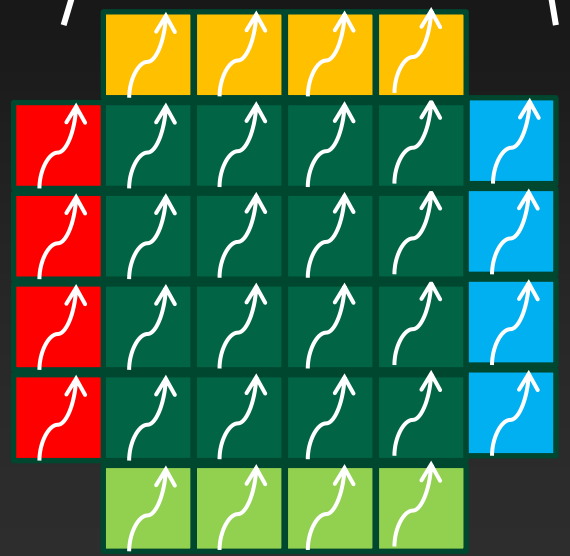


GPU Backend Overview

- Storage
  - IJK storage order
  - Coalesced reads in I direction
- Parallelization
  - Parallelize in IJ dimension (blocks are mapped to CUDA blocks)
  - Block boundary elements are updated using additional warps
- Data field indexing
  - Store data field pointers and strides in shared memory
  - Store indexes in registers



CUDA grid splits IJ plane into blocks

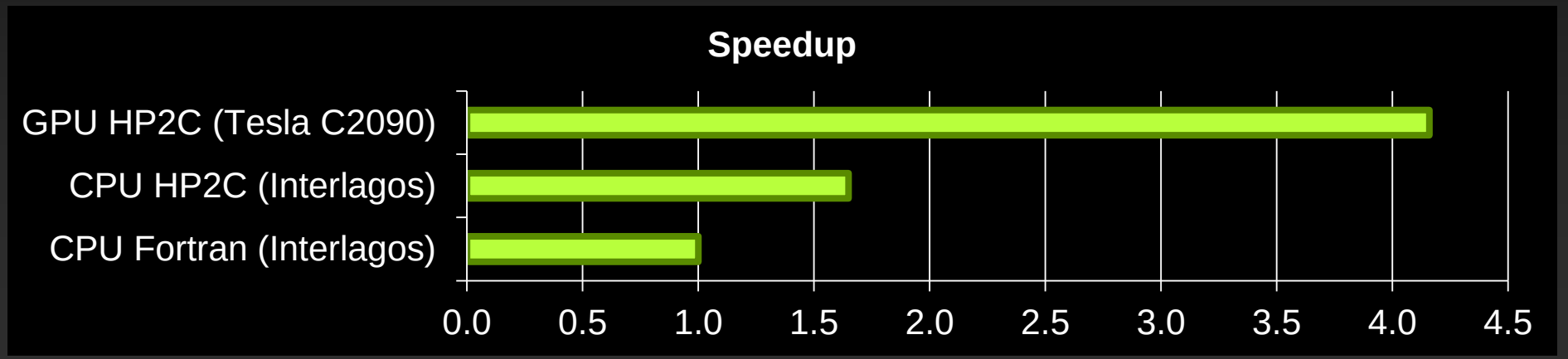


Block with boundary (use additional boundary warps)

HP2C Dycore Performance

- CPU / OpenMP Backend
  - Factor 1.6x – 1.7x faster than the standard COSMO implementation
  - Here: no SSE support (expect another 10% ~30% improvement)

- GPU / CUDA backend
  - Tesla M2090 (150 GB/s with ECC enabled) is roughly a factor 2.6x faster than Interlagos (16-Core Opteron CPU with 52 GB/s)
  - Ongoing performance optimization



Acceleration of Physical Parametrizations: Current State

- Parametrizations : processes not described by the dynamics, such as radiation or turbulence. Account for about 20 to 25 % of total runtime

- GPU versions of the parametrizations have been implemented in COSMO

- Currently implemented and tested physics:
  - Microphysics (Reinhardt and Seifert, 2006)
  - Radiation (Ritter and Geleyn, 1992)
  - Turbulence (Raschendorfer, 2001)
  - Soil (Heise, 1991)

- Account for 90-95% of physics in typical COSMO-2 run
- Only options for operational runs are supported
  - Unsupported features have been documented

Directives/Compiler choices for OPCODE

- OpenAcc: Open standard, supported by 3 compiler vendors PGI, Cray, Caps
  - Directives of choice for final OPCODE version
  - CAPS: Future approach

- PGI proprietary:
  - Enabled port of all kernels (some workarounds required)
  - First implementation of the physics
  - Translation to OpenAcc relatively straight forward

=> Testing code with different compilers can be very helpful!

```
!$acc parallel loop vector_length(N)
   do i=1,N
        a(i)=b(i)+c(i)
   end do
!$acc end parallel loop
```

Implementation in COSMO

- **Change to block data structure inside the physics**
  - **f(i,j,k) -> f_b(nproma,ke), with nproma = istartpar x iendpar / nblock.**
  - **nblock=1 for GPU run)**

- Physics loop restructured to iterate over blocks

```
transfer from CPU to GPU (ijk data f(i,j,k) )
!start block loop
   do ib=1,nblock
            call copy_to block
            call organize_gscp
            call organize_radiation
            call organize_turbulence
            call organize_soil
            call copy_back
   end do
transfer back GPU to CPU (ijk data f(i,j,k))
```

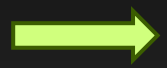
Required data on the GPU
All operations on grid data computed on the GPU
Physics timing region

inside physics scheme data is in block form
f_b(nproma,ke)

Porting Strategy for Parametrizations

- Pencil Parallelization: horizontal direction, 1 thread per vertical column
  - Most loop structures unchanged, one only adds directives
  - In some parts: loop restructuring to reduce kernel call overheads, and profit from cache reuse.
  - Remove NEC vector-optimization.

```
!$acc data present(a,c1,c2)
!vertical loop
do k=2,Nz
 !work 1
 !$acc parallel loop vector_length(N)
 do ip=1,nproma
  c2(ip)=c1(ip,k)*a(ip,k-1)
 end do
 !$acc end parallel loop
!work 2
!$acc parallel loop vector_length(N)
do ip=1,nproma
   a(ip,k)=c2(ip)*a(ip,k-1)
end do
!$acc end parallel loop
end do
!$acc end data
```

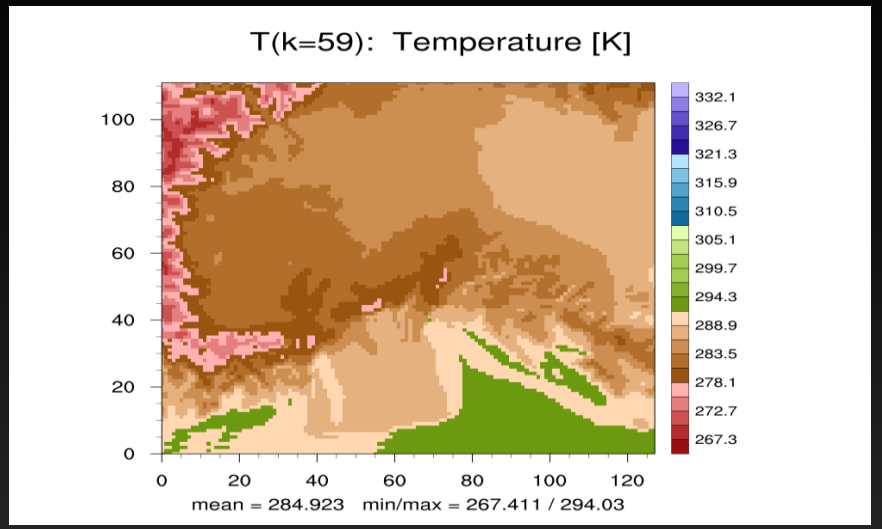


```
!$acc data present(a,c1)
!$acc parallel loop vector_length(N)
do ip=1,nproma
 !vertical loop
 do k=2,Nz
  !work 1
  c2=c1(ip,k)*a(ip,k-1)
  !work 2
   a(ip,k)=c2*a(ip,k-1)
 end do
end do
!$acc end parallel loop
!$acc end data
```

- Remove Fortran automatic arrays in subroutines which are often called (to avoid call to cudamalloc)
- Data regions to avoid CPU-GPU transfer
- Use profiler to target specific parts which need further optimization: reduce memory usage, replace intermediate arrays with scalars …

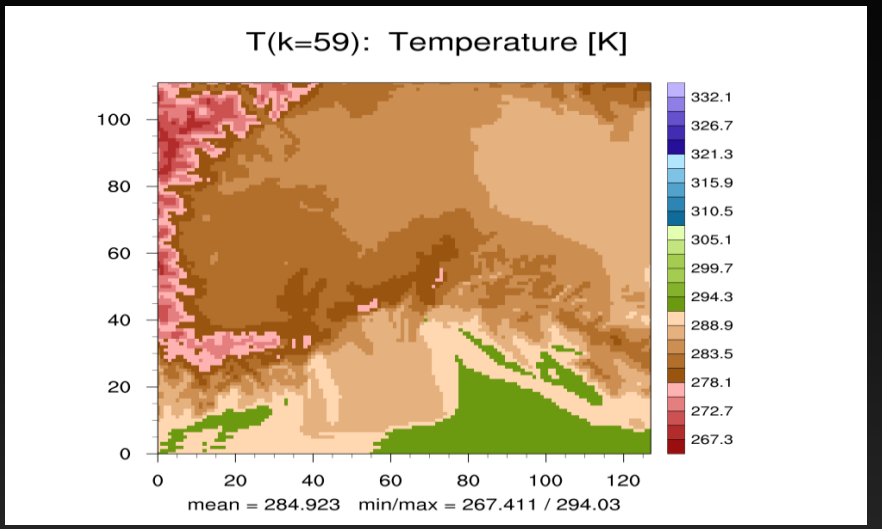
GPU/CPU comparison

CPU – original physics
16 cores (interlagos) – using MPI



Time physics: 42.4 s
(average time, without communication)

GPU – block physics
1 core + 1 GPU (X2090)



Time physics: 12.5 s

- Benchmark subdomain 128x112x60, 1h simulation with microphysics, radiation, turbulence and soil
- CPU-GPU results agree within roundoff error

GPU/CPU comparison, detail timing

	Original CPU time (s) 16 cores (Interlagos)	Block Physics GPU time (s) 1 core + 1 GPU (X2090)	Speed up
Microphysics	15.7 (37%)	2.3 (18%)	6.8x
Radiation	11.1 (26%)	2.6 (20%)	4.3x
Turbulence	14.4 (34%)	5.1 (41%)	2.8x
Soil	1.2 (3%)	0.5 (4%)	2.4x
Copy ijk ↔ block	-	2.0 (16%)	-
Total physics	42.4 (100%)	12.5 (100%)	**3.4x**

- Test subdomain 128x112x60, 1h simulation
- Currently running the block physics code on CPU (i.e. ignoring directives) is slower (total physics = 53 s). This is due to the GPU-loop reordering optimizations, not to the block structure. Having a single source code that runs efficiently on x86-CPU (i.e. excluding NEC) and GPU will require further work.
- The GPU code runs 7% faster on CASTOR (C2090)

Summary and next steps

- Dycore ported using portable stencil library and DESL
- Physics ported using directives

- Dycore speedup of ~4x vs original code
- Physics speedup of ~3.4x vs original code

- Dycore speedup for relevant domain sizes retained for K20/SandyBridge

- Ongoing: Combining Dycore, Physics and Messaging Layer


Thank you!
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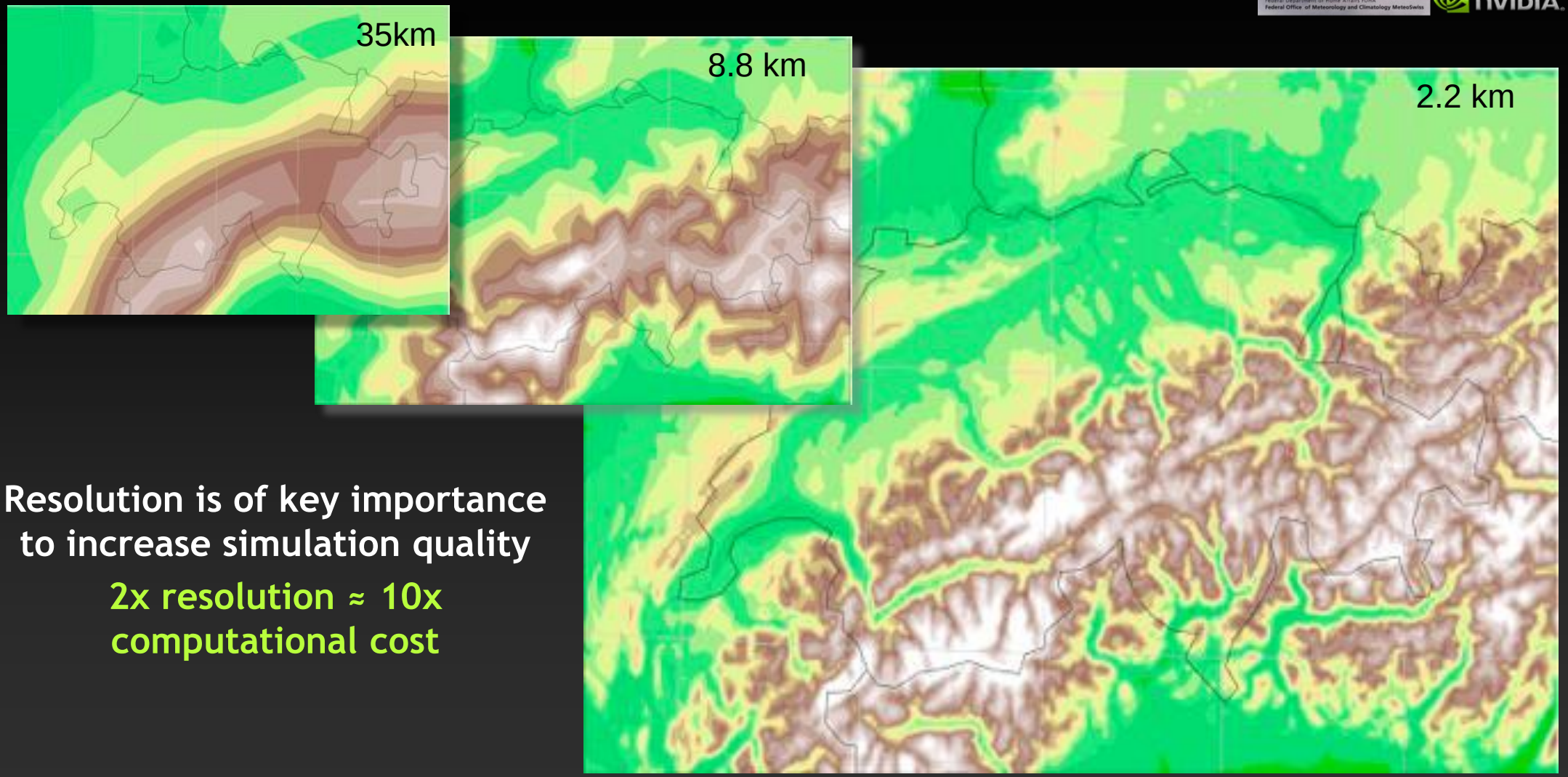
NVIDIA

Need for Higher Resolution in Switzerland



Resolution is of key importance to increase simulation quality

2x resolution ≈ 10x computational cost